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2-Methoxy-4-(prop-2-en-1-yl)phenyl 4-methoxybenzoate

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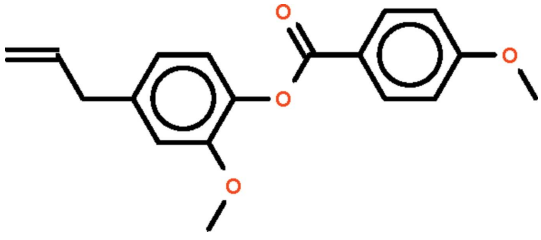
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.050; wR factor = 0.132; data-to-parameter ratio = 17.7.

In the title compound, $C_{18}H_{18}O_4$, the planes of the benzene rings are twisted by 81.60 (5)°. In the crystal, weak C—H···O hydrogen bonds link the molecules into supramolecular chains extending along the a axis.

Related literature

For the structure of phenyl benzoate, see: Shibakami & Sekiya (1995).



Experimental

Crystal data

$C_{18}H_{18}O_4$
M_r = 298.32
Triclinic, $P\overline{1}$
a = 8.7685 (6) Å
b = 9.8159 (7) Å
c = 10.3515 (6) Å
α = 113.030 (6)°
β = 101.231 (6)°
γ = 102.378 (6)°
V = 761.45 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.40 × 0.40 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.964, T_{max} = 0.982
6267 measured reflections
3525 independent reflections
2497 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.132
S = 1.06
3525 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18B···O3^{i}	0.98	2.54	3.458 (2)	156

Symmetry code: (i) $x+1, y, z$.

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5699).

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supplementary materials

Acta Cryst. (2013). E**69**, o819 [doi:10.1107/S1600536813011458]

2-Methoxy-4-(prop-2-en-1-yl)phenyl 4-methoxybenzoate

Mallikarjuna Rao Pichika, Beng Kang Yew and Seik Weng Ng

Comment

The title phenyl benzoate (Scheme I, Fig. 1), which possesses an allyl and a methoxy substituent, was synthesized for an evaluation of its pharmaceutical properties as it is an ester derivative of eugenol. The two benzene rings are approximately perpendicular [dihedral angle 81.60 (5)°]. The twist is similar to that found in the unsubstituted compound, phenyl benzoate (Shibakami & Sekiya, 1995). In the crystal, weak C—H···O hydrogen bond links molecules into the supramolecular chains extending along the a axis (Table 1).

Experimental

4-Allyl-2-methoxyphenol (1 mmol), 4-methoxybenzoic acid (1 mmol), diethylazodicarboxylate (2 mmol) and triphenylphosphine (2 mmol) were heated in THF (10 ml) for 2 h. The solid material extracted with dichloromethane. The dichloromethane solution was eluted through a silica gel column by using an *n*-hexane–ethyl acetate (95: 5 *v*/*v*) solvent system. Slow evaporation of the solution yielded large colorless crystals.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H 0.95 to 0.98 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO* (Agilent, 2013); data reduction: *CrysAlis PRO* (Agilent, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

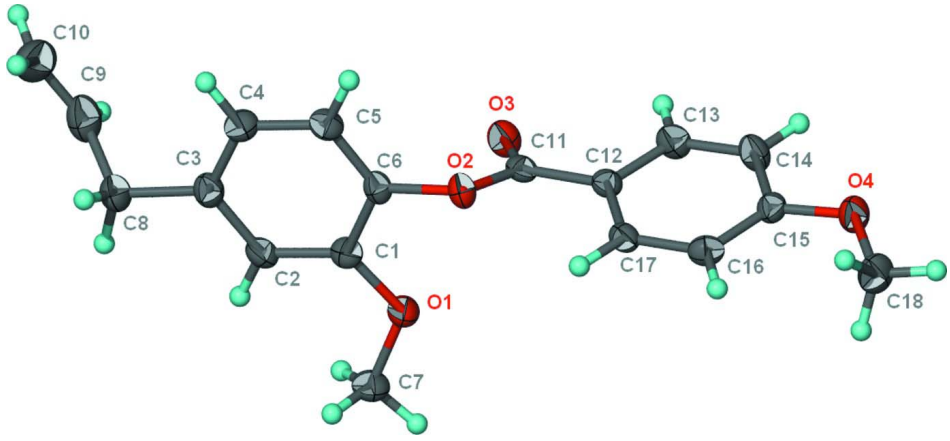

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{18}H_{18}O_4$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Methoxy-4-(prop-2-en-1-yl)phenyl 4-methoxybenzoate

Crystal data

$C_{18}H_{18}O_4$
M_r = 298.32
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.7685 (6) Å
b = 9.8159 (7) Å
c = 10.3515 (6) Å
α = 113.030 (6)°
β = 101.231 (6)°
γ = 102.378 (6)°
V = 761.45 (11) Å^3
Z = 2
$F(000)$ = 316
D_x = 1.301 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2058 reflections
θ = 3.4–27.5°
μ = 0.09 mm^{-1}
T = 100 K
Prism, colorless
0.40 × 0.40 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.964, T_{max} = 0.982
6267 measured reflections
3525 independent reflections
2497 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.6°, θ_{min} = 3.4°
h = −11→8
k = −11→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.132
S = 1.06
3525 reflections
199 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.0956P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.25854 (15)	0.56195 (13)	0.97044 (12)	0.0239 (3)
O2	0.17691 (14)	0.49329 (12)	0.68408 (12)	0.0201 (3)
O3	0.03197 (15)	0.26310 (13)	0.66616 (13)	0.0242 (3)
O4	0.54829 (15)	0.06265 (13)	0.33989 (13)	0.0245 (3)
C1	0.1367 (2)	0.61293 (18)	0.92258 (18)	0.0198 (4)
C2	0.0589 (2)	0.70167 (19)	1.01000 (18)	0.0212 (4)
H2	0.0890	0.7300	1.1126	0.025*
C3	−0.0628 (2)	0.75000 (19)	0.94958 (18)	0.0223 (4)
C4	−0.1092 (2)	0.70584 (19)	0.79870 (18)	0.0228 (4)
H4	−0.1929	0.7373	0.7565	0.027*
C5	−0.0329 (2)	0.61580 (19)	0.70993 (18)	0.0208 (4)
H5	−0.0646	0.5852	0.6069	0.025*
C6	0.0886 (2)	0.57120 (18)	0.77169 (17)	0.0186 (4)
C7	0.3292 (2)	0.6251 (2)	1.12758 (18)	0.0273 (4)
H7A	0.4173	0.5827	1.1487	0.041*
H7B	0.2443	0.5963	1.1700	0.041*
H7C	0.3742	0.7392	1.1712	0.041*
C8	−0.1423 (2)	0.8524 (2)	1.0485 (2)	0.0285 (4)
H8A	−0.0931	0.8723	1.1514	0.034*
H8B	−0.1166	0.9544	1.0460	0.034*
C9	−0.3225 (2)	0.7840 (2)	1.0064 (2)	0.0342 (5)
H9	−0.3629	0.6969	1.0236	0.041*
C10	−0.4308 (3)	0.8330 (3)	0.9476 (2)	0.0412 (5)
H10A	−0.3957	0.9198	0.9284	0.049*
H10B	−0.5447	0.7819	0.9239	0.049*
C11	0.1434 (2)	0.33704 (18)	0.64360 (17)	0.0181 (4)
C12	0.2555 (2)	0.27352 (18)	0.56621 (17)	0.0179 (4)
C13	0.2089 (2)	0.11166 (19)	0.47938 (18)	0.0232 (4)
H13	0.1070	0.0463	0.4717	0.028*
C14	0.3087 (2)	0.04630 (19)	0.40522 (19)	0.0241 (4)
H14	0.2745	−0.0635	0.3452	0.029*
C15	0.4596 (2)	0.14002 (19)	0.41746 (17)	0.0195 (4)
C16	0.5092 (2)	0.30149 (19)	0.50483 (18)	0.0210 (4)
H16	0.6126	0.3663	0.5146	0.025*
C17	0.4059 (2)	0.36649 (18)	0.57741 (17)	0.0193 (4)
H17	0.4387	0.4765	0.6357	0.023*
C18	0.7088 (2)	0.1525 (2)	0.3554 (2)	0.0301 (4)
H18A	0.7575	0.0844	0.2908	0.045*
H18B	0.7782	0.1986	0.4582	0.045*
H18C	0.7004	0.2360	0.3277	0.045*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0262 (7)	0.0270 (6)	0.0171 (6)	0.0127 (5)	0.0042 (5)	0.0077 (5)
O2	0.0243 (6)	0.0178 (6)	0.0196 (6)	0.0080 (5)	0.0107 (5)	0.0073 (5)
O3	0.0241 (7)	0.0222 (6)	0.0247 (7)	0.0046 (5)	0.0117 (5)	0.0085 (5)
O4	0.0221 (6)	0.0247 (6)	0.0262 (7)	0.0084 (5)	0.0119 (5)	0.0084 (5)
C1	0.0212 (9)	0.0180 (8)	0.0202 (9)	0.0055 (7)	0.0055 (7)	0.0096 (7)
C2	0.0226 (9)	0.0209 (8)	0.0157 (8)	0.0050 (7)	0.0050 (7)	0.0055 (7)
C3	0.0213 (9)	0.0214 (8)	0.0228 (9)	0.0062 (7)	0.0103 (7)	0.0075 (7)
C4	0.0223 (9)	0.0245 (9)	0.0225 (9)	0.0085 (7)	0.0054 (8)	0.0118 (7)
C5	0.0229 (9)	0.0227 (8)	0.0168 (8)	0.0057 (7)	0.0065 (7)	0.0095 (7)
C6	0.0205 (8)	0.0167 (8)	0.0188 (8)	0.0054 (7)	0.0091 (7)	0.0069 (7)
C7	0.0290 (10)	0.0306 (10)	0.0190 (9)	0.0110 (8)	0.0017 (8)	0.0098 (8)
C8	0.0293 (10)	0.0308 (10)	0.0227 (9)	0.0136 (8)	0.0096 (8)	0.0067 (8)
C9	0.0378 (12)	0.0304 (10)	0.0362 (11)	0.0124 (9)	0.0209 (10)	0.0114 (9)
C10	0.0325 (11)	0.0520 (13)	0.0377 (12)	0.0177 (10)	0.0126 (10)	0.0161 (10)
C11	0.0198 (8)	0.0185 (8)	0.0133 (8)	0.0050 (7)	0.0026 (7)	0.0062 (6)
C12	0.0182 (8)	0.0192 (8)	0.0152 (8)	0.0052 (7)	0.0047 (7)	0.0072 (6)
C13	0.0216 (9)	0.0206 (8)	0.0240 (9)	0.0024 (7)	0.0086 (8)	0.0084 (7)
C14	0.0266 (9)	0.0171 (8)	0.0244 (9)	0.0047 (7)	0.0103 (8)	0.0052 (7)
C15	0.0204 (8)	0.0229 (8)	0.0174 (8)	0.0102 (7)	0.0065 (7)	0.0094 (7)
C16	0.0178 (8)	0.0208 (8)	0.0226 (9)	0.0021 (7)	0.0045 (7)	0.0110 (7)
C17	0.0210 (9)	0.0165 (8)	0.0173 (8)	0.0052 (7)	0.0041 (7)	0.0060 (7)
C18	0.0219 (9)	0.0332 (10)	0.0345 (11)	0.0083 (8)	0.0148 (8)	0.0119 (8)

Geometric parameters (Å, º)

O1—C1	1.362 (2)	C8—H8A	0.9900
O1—C7	1.4381 (19)	C8—H8B	0.9900
O2—C11	1.3676 (19)	C9—C10	1.306 (3)
O2—C6	1.4110 (19)	C9—H9	0.9500
O3—C11	1.205 (2)	C10—H10A	0.9500
O4—C15	1.358 (2)	C10—H10B	0.9500
O4—C18	1.433 (2)	C11—C12	1.475 (2)
C1—C2	1.386 (2)	C12—C17	1.388 (2)
C1—C6	1.398 (2)	C12—C13	1.400 (2)
C2—C3	1.395 (2)	C13—C14	1.372 (2)
C2—H2	0.9500	C13—H13	0.9500
C3—C4	1.393 (2)	C14—C15	1.391 (2)
C3—C8	1.522 (2)	C14—H14	0.9500
C4—C5	1.389 (2)	C15—C16	1.396 (2)
C4—H4	0.9500	C16—C17	1.390 (2)
C5—C6	1.375 (2)	C16—H16	0.9500
C5—H5	0.9500	C17—H17	0.9500
C7—H7A	0.9800	C18—H18A	0.9800
C7—H7B	0.9800	C18—H18B	0.9800
C7—H7C	0.9800	C18—H18C	0.9800
C8—C9	1.478 (3)		

C1—O1—C7	116.79 (13)	C10—C9—C8	125.6 (2)
C11—O2—C6	116.91 (13)	C10—C9—H9	117.2
C15—O4—C18	117.48 (13)	C8—C9—H9	117.2
O1—C1—C2	125.77 (15)	C9—C10—H10A	120.0
O1—C1—C6	115.87 (14)	C9—C10—H10B	120.0
C2—C1—C6	118.36 (15)	H10A—C10—H10B	120.0
C1—C2—C3	120.95 (16)	O3—C11—O2	122.70 (15)
C1—C2—H2	119.5	O3—C11—C12	125.80 (15)
C3—C2—H2	119.5	O2—C11—C12	111.46 (14)
C4—C3—C2	119.50 (16)	C17—C12—C13	118.63 (15)
C4—C3—C8	120.39 (16)	C17—C12—C11	123.04 (14)
C2—C3—C8	120.10 (15)	C13—C12—C11	118.32 (15)
C5—C4—C3	119.97 (16)	C14—C13—C12	120.75 (16)
C5—C4—H4	120.0	C14—C13—H13	119.6
C3—C4—H4	120.0	C12—C13—H13	119.6
C6—C5—C4	119.76 (15)	C13—C14—C15	120.34 (15)
C6—C5—H5	120.1	C13—C14—H14	119.8
C4—C5—H5	120.1	C15—C14—H14	119.8
C5—C6—C1	121.45 (15)	O4—C15—C14	115.22 (14)
C5—C6—O2	119.49 (14)	O4—C15—C16	125.00 (15)
C1—C6—O2	118.84 (14)	C14—C15—C16	119.78 (15)
O1—C7—H7A	109.5	C17—C16—C15	119.31 (15)
O1—C7—H7B	109.5	C17—C16—H16	120.3
H7A—C7—H7B	109.5	C15—C16—H16	120.3
O1—C7—H7C	109.5	C12—C17—C16	121.17 (15)
H7A—C7—H7C	109.5	C12—C17—H17	119.4
H7B—C7—H7C	109.5	C16—C17—H17	119.4
C9—C8—C3	114.01 (15)	O4—C18—H18A	109.5
C9—C8—H8A	108.8	O4—C18—H18B	109.5
C3—C8—H8A	108.7	H18A—C18—H18B	109.5
C9—C8—H8B	108.7	O4—C18—H18C	109.5
C3—C8—H8B	108.7	H18A—C18—H18C	109.5
H8A—C8—H8B	107.6	H18B—C18—H18C	109.5

C7—O1—C1—C2	−9.9 (2)	C3—C8—C9—C10	−109.0 (2)
C7—O1—C1—C6	169.69 (14)	C6—O2—C11—O3	8.1 (2)
O1—C1—C2—C3	178.83 (15)	C6—O2—C11—C12	−173.97 (12)
C6—C1—C2—C3	−0.8 (2)	O3—C11—C12—C17	−161.98 (17)
C1—C2—C3—C4	1.3 (3)	O2—C11—C12—C17	20.1 (2)
C1—C2—C3—C8	−177.75 (16)	O3—C11—C12—C13	17.0 (2)
C2—C3—C4—C5	−0.7 (3)	O2—C11—C12—C13	−160.88 (14)
C8—C3—C4—C5	178.28 (15)	C17—C12—C13—C14	−0.9 (3)
C3—C4—C5—C6	−0.3 (3)	C11—C12—C13—C14	−179.88 (15)
C4—C5—C6—C1	0.7 (3)	C12—C13—C14—C15	1.2 (3)
C4—C5—C6—O2	−173.71 (14)	C18—O4—C15—C14	−176.50 (15)
O1—C1—C6—C5	−179.87 (15)	C18—O4—C15—C16	3.6 (2)
C2—C1—C6—C5	−0.2 (2)	C13—C14—C15—O4	179.68 (16)
O1—C1—C6—O2	−5.4 (2)	C13—C14—C15—C16	−0.5 (3)
C2—C1—C6—O2	174.27 (14)	O4—C15—C16—C17	179.26 (15)

C11—O2—C6—C5	−107.13 (17)	C14—C15—C16—C17	−0.6 (2)
C11—O2—C6—C1	78.29 (18)	C13—C12—C17—C16	−0.2 (2)
C4—C3—C8—C9	59.1 (2)	C11—C12—C17—C16	178.76 (15)
C2—C3—C8—C9	−121.88 (19)	C15—C16—C17—C12	0.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18*B*···O3^{i}	0.98	2.54	3.458 (2)	156

Symmetry code: (i) *x*+1, *y*, *z*.